The calculation of thermodynamic properties from Song and Mason equation of state

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Introduction

Recent work by Song and Mason on a statistical-mechanical theory for the equation of state of fluids has yielded simple but remarkably accurate results for both spherical [1] and molecular [2] fluids. The purpose of this work is to apply this equation of state to calculate thermodynamic properties of argon.

Theory

Song and Mason [2] obtained an analytical equation of state for convex-molecule fluids based on statistical-mechanical perturbation theory. The equation of state is of the form,

\[ \frac{P}{\rho kT} = 1 + \frac{1}{B_2(T)} [\alpha(T)\rho \{ G(\eta) - 1 \} + \phi(T)\rho^2] \]  

(1)

where \( P \) is the pressure, \( \rho \) is the molar (number) density, \( B_2(T) \) is the second virial coefficient, \( \alpha(T) \) is the contribution of the repulsive forces to the second virial coefficient, \( G(\eta) \) is the average pair distribution function at contact for equivalent hard convex bodies, and \( kT \) has its usual meaning. The adopted form for \( G(\eta) \) have been defined in Ref. 2.

The equation of state has been applied to calculate thermodynamic properties including the fugacity coefficient, the enthalpy, the entropy, and the speed of sound for argon. The correlations for these calculations have been defined in Ref. 3.
Result

Our calculated results on the fugacity coefficient, enthalpy, entropy and speed of sound are in very good agreement with the experimental values in Ref. 4 and 5. The results are shown in figures 1-3 and the maximum deviations of the calculated isobars of the speed of sound compared with the experimental data in Ref. 5 extend to ± 8%.

Figure 1. The plot of fugacity coefficient, $f/P$, as a function of pressure at 110 K (•), 150 K (∇), 200 K (♦), and 400 K (◊). The curves (solid lines) represent the equation of state, and the points are taken from Ref. 4.

Figure 2. The plot of enthalpy, $H$, as a function of temperature at 1 bar (•), 50 bar (∇), 100 bar (♦), and 200 bar (◊). The curves (solid lines) represent the equation of state, and the points are taken from Ref. 5.

Figure 3. The plot of entropy, $S$, as a function of temperature at 1 bar (•), 50 bar (∇), 200 bar (♦), 500 bar (◊). The curves (solid lines) represent the equation of state, and the points are taken from Ref. 5.
References
